A ROUGHENING TRANSITION INDICATED BY THE BEHAVIOUR OF GROUND STATES

R. Kotecký and S. Miracle-Sole

Dept. of Mathematical Physics, Charles University, V. Holesovickách 2
18000 - Praha 8 - Czechoslovakia
Centre de Physique Théorique, CNRS Luminy, Case 907,
F-13288 Marseille Cedex 9, France

ABSTRACT

Our aim in this contribution is to present some illustrations for the claim that already by looking at the ground states of classical lattice models, one may meet some interesting and non-trivial structures.

KEYWORDS: Roughening transition, Ising spin systems, BCC lattice, equilibrium crystal.

First of all we shall clarify what we mean by ground states. We consider a finite spin model on a lattice $\mathcal{L}$ with configuration space $\Omega = S^{\mathcal{L}}$ and finite range interaction $\{\varphi_\Lambda, \Lambda \subset \mathcal{L}\}$. The energy in a finite volume $V \subset \mathcal{L}$, under a boundary condition (b.c.) $\bar{\sigma} \in \Omega$ is, in an obvious notation,

$$H_V(\sigma_V \mid \bar{\sigma}) = \sum_{\sigma_V : V \cap \Lambda \neq \emptyset} \varphi_\Lambda(\sigma_V \cup \bar{\sigma}_V)$$

The collection of finite volume Gibbs states (a specification)

$$\mu_V^{\beta H}(\sigma_V \mid \bar{\sigma}) = Z_V(\bar{\sigma})^{-1} \exp\left(-\beta H_V(\sigma_V \mid \bar{\sigma})\right)$$

where

$$Z_V(\bar{\sigma}) = \sum_{\sigma_V} \exp\left(-\beta H_V(\sigma_V \mid \bar{\sigma}\right)$$

determine (by the DLR equations) the set $G(\beta H)$ of the Gibbs measures on $\mathcal{L}$ corresponding to a hamiltonian H and an inverse temperature β. If a Gibbs state $\mu \in G(\beta H)$ happens to equal the limit

$$\mu = \lim_{V \uparrow \mathcal{L}} \mu_V^{\beta H}(\cdot \mid \bar{\sigma})$$

under a fixed b.c. $\bar{\sigma}$, we shall call it Gibbs state corresponding to a b.c. $\bar{\sigma}$.

Following Dobrushin and Schlosman [1] we introduce the ground states simply as the Gibbs states at $\beta = \infty$; i.e. as the Gibbs states determined by the specification

$$\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}) = \lim_{\beta \to \infty} \mu_V^{\beta H}(\sigma_V \mid \bar{\sigma})$$

Clearly

$$\mu_V^{\infty H}(\sigma_V \mid \bar{\sigma}) = \begin{cases} 1/|M_V(\bar{\sigma})| & \text{if} \quad \sigma_V \in M_V(\bar{\sigma}) \\ 0 & \text{if} \quad \sigma_V \notin M_V(\bar{\sigma}) \end{cases}$$

where

$$M_V(\bar{\sigma}) = \{\tilde{\sigma}_V \mid H_V(\tilde{\sigma}_V \mid \bar{\sigma}) = \inf_{\sigma_V} H_V(\sigma_V \mid \bar{\sigma})\}$$

is the set of ground configurations in V under the b.c. $\bar{\sigma}$. A ground state will be called rigid if it is supported by a single configuration $\sigma \in \Omega$, i.e. if it is a Dirac measure δ_σ on Ω. However, the ground states may often be measures supported by a large set of configurations. Examples of such random ground states are met e.g. for the Ising antiferromagnet on triangular or FCC lattices. We notice that even the problem of describing all the extremal periodic ground states is often non trivial. Let us mention in this connection the case of the three state Potts antiferromagnet on a square or cubic lattice which is still open. An attempt to clarify it by mapping the ground states onto the Gibbs states of equivalent ferromagnetic models at a particular temperature was made in [2].

Of course, an important problem is to distinguish which ground states are stable in the sense that there exist Gibbs states at low temperature that are "near" to the ground states in question. Some particular cases of periodic rigid ground states are covered by the Pirogov-Sinaï theory [3] and a a class of non translation invariant rigid ground states was tackled in [4]. A general criterium for the stability of rigid ground states has been conjectured by Dobrushin and Shlosman [1]. However, no theory of stability exists for random ground states, although some statements about the thermodynamics involving such ground states were proven in a work by Aizenman and Lieb [5] about the third thermodynamical principle.

When probing Gibbs states at low temperatures a useful notion may be thet of <u>weak ground states</u> [1] describing the effect of small perturbation added to the hamiltonian. Namely, considering an additional finite range interaction $\{\tilde{\varphi}_\Lambda\}$ and the corresponding hamiltonian $\tilde{H}$, a weak ground state (corresponding to the "direction" $\tilde{H}$) is a Gibbs state with the specification

$$\mu_V^{\infty H,\tilde{H}}(\sigma_V \mid \bar{\sigma}) = \lim_{\beta\to\infty} \mu_V^{\beta(H+\tilde{H}/\beta)}(\sigma_V \mid \bar{\sigma}) =$$

$$\begin{cases} = \dfrac{\exp -\tilde{H}_V(\sigma_V \mid \bar{\sigma})}{\sum\limits_{\sigma_V\in M_V(\bar{\sigma})} \exp -\tilde{H}_V(\sigma_V \mid \bar{\sigma})} & \text{if} \quad \sigma_V \in M_V(\bar{\sigma}) \\ = 0 & \text{if} \quad \sigma_V \notin M_V(\bar{\sigma}) \end{cases}$$

Let us now inspect two particular exemples with an interesting structure of weak ground states. The case of periodic ground states will be discussed for an Ising antiferromagnet in an external magnetic field [1,6], while our main exemple, the ground states describing an interface and its roughening, will be discussed for an Ising model on a BCC lattice.

Considering the Ising antiferromagnet on a square lattice with a nearest neighbour (n.n.) coupling J and an external field h, one easily shows that, for $|h| < 4|J|$ there are the two customary antiferromagnetic rigid ground states (stable according to, say the Pirogov-Sinaï theory). Inspecting now the border points, say $h = 4|J|$, we get random ground states living on the set of all configurations for which no nearest neighbours are occupied by a pair of minus spins. Following [1,6] we may look at the lattice sites with minus spins as is they were occupied by a particle and thus we may equivalently think of a hard core lattice gas. Considering now the limit $\beta \to \infty$ along the lines $h = 4|J| + \mu/\beta$ as shown in Fig. 1, i.e. a weak ground states in the direction $\tilde{H}$ given by the external field μ, we get a hard core lattice gas with a chemical potential -2μ, which is expected to have a critical value $\mu_c \sim -(1/2)\ln 3.8$ (for a rigorous estimate see [6]). This suggest the phase diagram of Fig. 1.

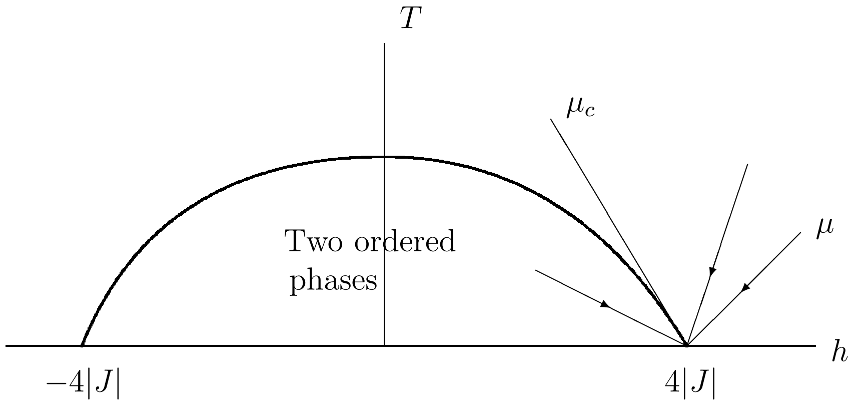

Fig. 1

Finally, let us consider the case of an Ising model on a BCC lattice with a n.n. ferromagnetic coupling $J_0 > 0$ and a n.n.n. coupling J. Let us stress right now that we have in mind an isotropic model. Whenever $J > -(2/3)J_0$ there are two stable, rigid, translation invariant ground states of constant magnetization. We shall enforce the (100) interface between these two phases by taking a b.c. $\bar{\sigma}$ with $\bar{\sigma}_i = +1$ if $i = (i_1, i_2, i_3)$ is a lattice site with $i_1 \leq 0$ and $\bar{\sigma}_i = -1$ if $i_1 < 0$. For $J > 0$ it is easy to show that such b.c. leads to a rigid ground state supported by $\bar{\sigma}$ itself. Using the method of Dobrushin [8] as generalized in [4] or the method of van Beijeren [9], one may prove that this ground state is stable; actually one gets the existence of the corresponding Gibbs state with a rigid interface in all the region shaded in Fig. 2 (with $\alpha_0 = (1/2)\ln(1+\sqrt{2})$) denoting the critical value for the Ising model on a square lattice. A more interesting situation is obtained for $J = 0$. Let us consider right away the weak ground states corresponding to the directions $\bar{H}$ yielded by a n.n.n. interaction of the form $J = \alpha/\beta$, i.e. the weak ground states obtained along the lines shown in Fig. 2. One easily observes that the configurations in $M_V(\bar{\sigma})$ contain interfaces with no overhands. Actually these configurations are exactly those considered by van Beijeren in his body centered solid-on-solid (BCSOS) model [10]. Without going into the details [7] we may refer to his results to get a description of our weak ground states in terms of a six vertex model with the weights $\omega_1 = \omega_2 = \omega_3 = \omega_4 = e^{-\alpha}$, $\omega_5 = \omega_6 = 1$. If $\alpha > \alpha_R = (1/2)\ln 2$, the six-vertex model is in the ferroelectric phase and the interface is rigid; if $\alpha < \alpha_R$, the results about the six-vertex model are usually interpreted as describing a rough interface wich actually should mean that the corresponding infinite volume Gibbs state of the BCSOS model thus not exist and our weak ground state is translation invariant. Even though the above equivalence is exact only in the limit $\beta \to \infty$, one may expect that there is a curve $T_R(J)$ of roughening transitions as shown in Fig. 2.

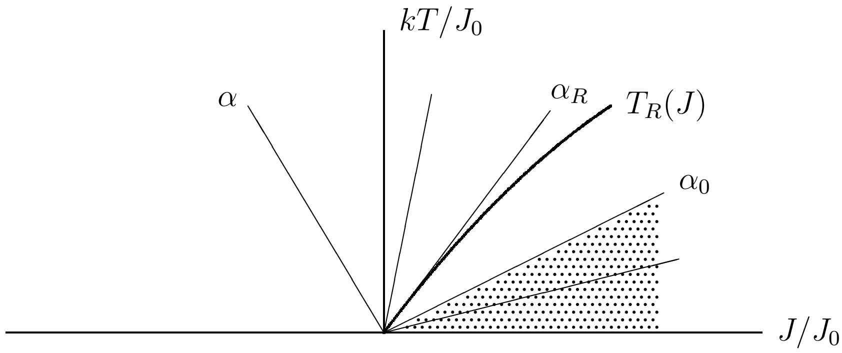

Fig. 2

Let us mention that one may investigate also the ground states with other b.c. $\bar{\sigma}(\vec{k})$ corresponding to general inclined interfaces (k_1, k_2, k_3) with normal $\vec{k}$. It turns out that for both positive and negative J the ground state corresponding to an interface (110) is rigid and stable while the ground state corresponding to an interface (111) is translation invariant and the interface is rough. To see this fact one may (for any J in an interval around zero) use a sililar equivalence as above to the triangular Ising solid on solid (TISOS) model and then refer to the analysis of this model by Nienhuis, Hilhorst and Blöte [11] who solved it exactly. When one of the conditions $-k_1 \le k_2 + k_3 \le k_1$, $-k_2 \le k_3 + k_1 \le k_2$ or $-k_3 \le k_1 + k_2 \le k_3$ is fulfilled the interface corresponding to the b.c. $\bar{\sigma}(\vec{k})$ is again described in terms of a BCSOS model with the appropriate b.c. which is, in its turn, equivalent to a six vertex model with fixed polarizations. For normals $\vec{k}$ in the complementary region the corresponding interface may be described in terms of a TISOS model.

To conclude let us comment about the connection of the roughening transition in the above sense and the facet formation in the equilibrium shape of a crystal (a droplet in the Ising model). One expects (see for instance [12]) that the roughening transition corresponds to the rounding of facets while a rigid interface associated to the b.c. $\bar{\sigma}(\vec{k})$ would imply the presence of a cusp in the corresponding direction in the graph of the surface tension as a function of $\vec{k}$, and by the Wulff construction give rise to a plane facet. In fact following Bricmont, El Mellouki and Fröhlich [12] one may use correlation inequalities to prove the existence of a cusp for the (100) facet in the shaded region of Fig. 2 and for the (110) facet if T is small enough and $J \geq 0$. In what concerns the rounding of the facets some insight may be obtained by introducing the free energy

$$f_V(\vec{k}) = S_V^{-1} \ln Z^{\mathrm{SOS}}(S_V, \vec{k})$$

of the appropriate SOS model and b.c. associated as explained above to the b.c. $\bar{\sigma}(\vec{k})$ of the Ising model in the volume V (S_V denoting the area of the interface (k_1, k_2, k_3) let $e_V(\vec{k})$ denote the energy of the corresponding ground state per unit area. Then, for finite volumes, one may show that the surface tension of the Ising model

$$\tau_V(\vec{k}) = S_V^{-1} \ln \left(Z(V, \vec{k}) / Z^+(V) \right)$$

behaves asymptoticaly with $T \to 0$ as

$$\tau_V(\vec{k}) = e_V(\vec{k}) + kT f_V(\vec{k})$$

Supposing that this is correct also in the thermodynamic limit, the function $\tau_V(\vec{k})$ con in principle be computed using the equivalence of the SOS models with b.c. with exact solvables models with fixed polarizations and from it get quantitative information on the equilibrium crystal shape as a function of the coupling constants.

Note:

The present text, publised in *VIIIth International Congress on Mathematical Physics*, M. Mebkhout and R. Sénéor editors, World Scientific, Singapore, 1987 (ISBN 9971-50-208-9), pp. 331–337, is our contribution to this conference, held in Marseille, France, July 16–25, 1986.

This congress, organized by the International Association of Mathematical Physics, belongs to a series, that begun in 1972 at Moscow and has been pursued in 1974 at Warsaw, 1975 Kyoto, 1977 Roma, 1979 Lausanne, 1981 Berlin, and 1983 Boulder. After Marseille, the congress took place at Swansea, in 1988.

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